Schottky Barrier Carbon Nanotube FET (CNTFET) Gas Sensors

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Abstract

In Schottky barrier (SB) carbon nanotube field effect transistors (CNTFET), work function of source/drain metal decides the behavior of the device. Using atomistic simulations, we find that Au, Pt, Pd contact results in NFET, PFET and ambipolar device respectively. Further, we see that NO_2 adsorbed on CNT results in p-type semiconductor with higher carrier density and conductance than the intrinsic CNT.

1. Introduction

Carbon nanotubes (CNTs) have unique electron transport, ideal channel properties and very sharp response in high speed and low power electronics [1]. In CNTFETs, metal-CNT contact determines the electron transport through a CNT [1-2]. The performance of the CNTFET is mostly controlled by the factors like, Schottky barrier (SB) and work function of the metal (Φ_m) used as source/drain contacts [3]. In SB-CNTFETs source/drain regions are two metal pads and semiconducting CNT is present between them acting as channel [3-4]. Geometrically two SB diodes are formed: source-CNT and drain-CNT [5]. Single walled (SW) CNT in channel region can interact with gas molecules, inducing an interfacial dipole that changes the Φ_m and height of the SB at the contacts, thus results in change in the output characteristics [6-7]. Thus the role of various metals in SB formation and its impact on the device characteristics is an import issue needing an investigation. In this study, we designed SB-CNTFET by using ATK Quantum wise package [8]. Using this tool, we can define various metal contacts, CNTs, gas molecules and crystals. In these devices ballistic transport is assumed by ignoring scattering of electrons [9].

2. SB-CNTFET and Role of Metal Work Function Φ_m

We designed a back-gated CNTFET as shown in the Fig. 1(a), 2(a) and 3(a) for three different metals gold (Au), platinum (Pt) and palladium (Pd). The design specifications of SB-CNTFETs are: surface cleavage (1 1 0) used for Au, Pt and Pd for quick optimization, zigzag CNT Chirality of (10, 0) acting as semiconducting channel. Gate metal is Aluminum. The gate dielectric is high-K material HfO_2 (hafnium oxide) with 1nm thickness. Length of the channel is 4 nm, which is limited by computational resources.

The carrier transport in CNTFETs is due to direct tunneling of carriers through the barrier. This phenomenon is called Field emission [2]. Based on the Φ_m and work function of CNT (Φ_{CNT}) following three cases arise: 1) if $\Phi_m > \Phi_{CNT}$, then CNTFET acts as PFET because the Fermi level of source metal is near to the valence band of CNT. If negative gate voltage is applied, CNT bands will bend and the valence band of CNT line ups exactly with metal Fermi level. Then narrow SB is established between metal Fermi level and valence band of CNT, leading to holes tunneling through this barrier by applying negative drain voltage [2]. 2) Similarly, if $\Phi_m < \Phi_{CNT}$, then it acts as NFET, where conduction band of CNT lines up exactly with metal Fermi level. 3) If the Fermi level of metal exactly line ups with the Fermi level of CNT, then the device acts as ambipolar. For positive bias, electrons will tunnel through the barrier and for negative bias holes will tunnel through the barrier.

3. Results and Discussions

The work functions Φ_m of three metals are shown in table 1. In Au-contacted CNTFET, $\Phi_{Au} < \Phi_{CNT}$. Thus the device should work like an NFET, this is confirmed by I-V characteristics in Fig. 1(b). Initially the metal Fermi level is near to the conduction band of CNT, on applying the positive gate bias the SB width will start decreasing and carrier tunnel from source to drain. As we increase gate voltage the band bending is also high, resulting in the Fermi level of metal to exactly line up with the conduction band of CNT thus more electrons cross the barrier and current increases. In Fig. 1(b) current is 0 A at V_{ds} = 0V then linearly increases from V_{ds} = 0.2 V to 0.4 V and then slowly enters into saturation beyond 0.4 V. Similarly, in Pt contacted CNTFET, $\Phi_{Pt} > \Phi_{CNT}$ as shown in table 1, and thus acts as PFET whose characteristics are shown in Fig. 2(b).

In Pd contacted CNTFET, $\Phi_{Pd} \leq \Phi_{CNT}$. From our study this device acts as NFET because of lesser work function than CNT, and also it can act as ambipolar device with dominant NFET characteristics. In this, the SB width is very high as shown in table. 1, so it is very difficult for the electrons to tunnel through the barrier, results in low drain current. This property highlights the effect of SB on CNTFET as shown in Fig. 3(b). For V_{gs} =1.0V, we observe one local minima and maxima at V_{ds} of 0.25V and 0.35V respectively, explained with the help of transmission spectrum T (E) shown in Fig. 4. T (E) gives transmission factor of carriers for different energies. For V_{ds} = 0.25V, T (E) shows that Fermi level moves towards valence band, at this point transmission factor has a peak value, which is symmetric. So, transmission of electrons and holes across the Fermi level is nearly equal resulting in a minimum. At V_{ds} = 0.35V, Fermi level moves deeper into valence band and transmission of holes is high compared to electrons across

Table I. Metals and their work functions

Metals	Φ_m (eV)	$\Phi_m - \Phi_{CNT}$ (Φ_{CNT} 5.6716)
Platinum (Pt)	5.905	0.2334
Palladium (Pd)	5.504	-0.1676
Gold (Au)	5.3877	-0.2839

the Fermi level. So transmission is dominant due to holes, resulting in local maxima. Further, we study the devices for gas sensing applications. The I-V characteristics of NO_2 adsorbed CNTFET is shown in Fig. 5(a). When NO_2 molecules are adsorbed on the bare CNT, it results in channel to behave as p-type semiconductor with higher carrier density, which is explained by density of states (DOS) shown in Fig. 5(b). This reveals that there is change in Fermi level of CNT, thus resulting in shift in Φ_{CNT}. Then the barrier between the source and channel will modulate accordingly and it will change the output characteristics as shown in Fig. 6. Further we note that the gas molecule at the source end increases the barrier width and vice versa on the drain side. The difference is high in saturation region that is beyond 0.4V.

4. Conclusions
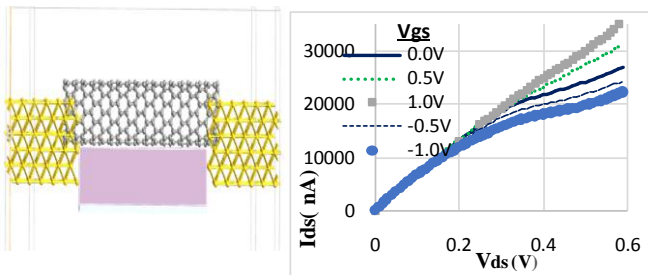
We study SB-CNTFET and find that it can act as PFET as well as NFET based on the type of metal used in source/drain contacts. Au and Pt contacted CNTFET acts as NFET and PFET respectively with high currents. Pd-CNTFET acts as ambipolar device and it reveals the effect of SB on drain currents. Further, we find that NO_2 adsorbed on CNT converts the channel from intrinsic to p-type, thus changing the channel conductivity and is helpful to detect the gas. It is noted that in saturation region the device is highly sensitive to the gases adsorbed.

References
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Fig. 1. a) CNTFET with Gold contacts. b) I_{ds} vs V_{ds} characteristics of Au-CNTFET for different V_{gs}.

Fig. 2 a) CNTFET with platinum contacts b) I_{ds} vs V_{ds} characteristics of Pt-CNTFET for different V_{gs}.
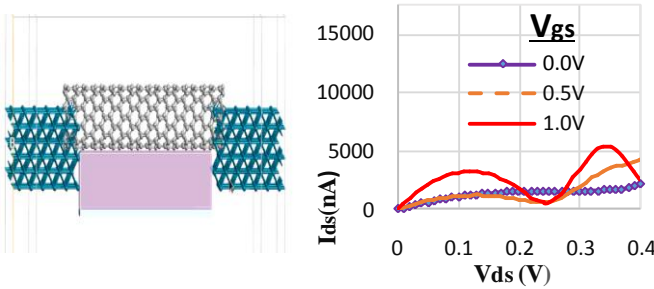

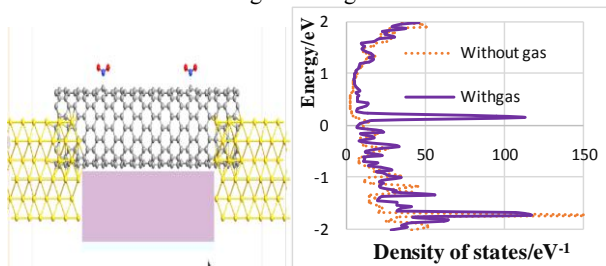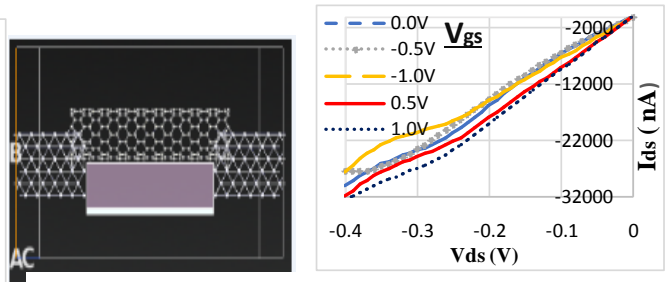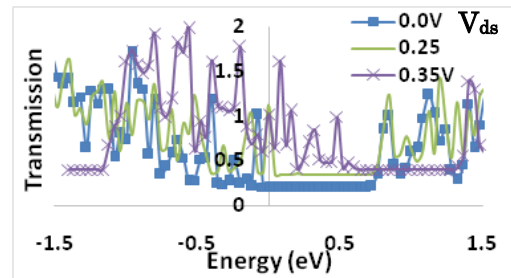Fig. 3(a) CNTFET with Palladium contacts, b) I_{ds} vs V_{ds} characteristics for different gate voltages and effect of SB.

Fig. 4 Transmission characteristics of CNTFET with Pd contact at V_{GS} = 1.0V and for V_{DS} = 0V, 0.25V and 0.35V

Fig 5. a) Au-CNTFET with two NO_2 gas molecule optimized on it. b) Density of states of CNT(Channel) in CNTFET with and without NO_2 gas, where fermilevel (E_f) is at E=0 eV.
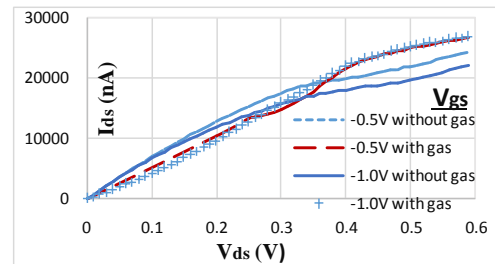

Fig. 6 Comparison of output characteristics of Au contacted CNTFET with and without NO_2 gas at V_{GS} = - 0.5V and -1.0V.